

Path Integral Formulation of Anomalous Diffusion Processes

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(Dated: October 27, 2011)

We present the path integral formulation of a broad class of generalized diffusion processes. Employing the path integral we derive exact expressions for the path probability densities and joint probability distributions for the class of processes under consideration. We show that Continuous Time Random Walks (CTRWs) are included in our framework. A closed expression for the path probability distribution of CTRWs is found in terms of their waiting time distribution as the solution of a Dyson equation. As the formalism naturally includes the treatment of functionals a generalized Feynman-Kac formula is derived.

PACS numbers: 05.40.Fb, 05.10.Gg, 52.65.Ff

Introduction: In addition to Langevin equations and Fokker-Planck equations, the concept of path integrals plays a central role in the description of stochastic processes [1, 2]. The path integral formulation is based on the specification of a probability measure assigned to each realization of the process and, hence, encodes the complete statistical information on the process. It was pioneered by Onsager and Machlup who derived an expression for the probability density of a path of a linear Gaussian process [3]. Later their work has been extended to include nonlinear drift and diffusion coefficients as well as coloured noise [4].

Despite the success of models based on Brownian motion and diffusion processes, over the last two decades it has become apparent that many dynamical systems in diverse fields, ranging from biology to physics, cannot aptly be described within this framework [5–7]. Various generalizations of diffusion processes have been considered to account for such anomalous diffusion. Some of these generalized models consist of an additional stochastic process. Examples include the Continuous Time Random Walk (CTRW) [8] which has been applied to model a variety of different systems [6]. The CTRW is defined as a proper random walk with an additional random process governing the waiting time between successive jumps. If the waiting time distribution is assumed to be scale-free the CTRW can be described by the celebrated fractional Fokker-Planck equation (For a review, we refer the reader to [6]). The corresponding Langevin equation can be formulated by application of the concept of subordination [9]. A path integral formulation of CTRWs has not been established so far. Such a formulation, however, is of particular importance since CTRWs in general are non-Markovian processes and as such insufficiently described by single-point probability distributions [10]. Another example where stochastic dynamical processes are combined with an additional random process is the field of

superstatistics [11].

This Letter presents a path integral approach to diffusion processes which are additionally driven by a further stochastic process. This class of processes comprises the CTRW and thus fills the gap of the lacking path integral formulation for CTRW's.

Path integral representation: The class of processes under consideration in this Letter is defined by the one-dimensional discrete Langevin equation

$$q_{k+1} = q_k + \tau N(q_k) + \sqrt{\tau D} R_k + \alpha_k r_k, \quad (1)$$

where the first three terms on the right hand side describe a standard Langevin equation with time step τ , drift $N(q_k)$ and Gaussian random variables R_k with amplitude \sqrt{D} . The anomalous contribution stems from the last term where α_k and r_k both are random variables. The transition amplitude of this process can be obtained as

$$p(q_{k+1}|q_k, \alpha_k) = \int \frac{d\tilde{q}_k}{2\pi} e^{i\tilde{q}_k(q_{k+1}-q_k-\tau N(q_k)-\alpha_k r_k)-\frac{\tau D}{2}\tilde{q}_k^2}, \quad (2)$$

where we assumed the stochastic force R_k to be Gaussian distributed with zero-mean and vanishing correlation $\langle R_k R_l \rangle = \delta_{jk}$. The probability for a path starting at q_0 is given by iteration of Eq.(2)

$$g_{k+1}(q_{k+1}; q_k, \alpha_k; \dots, q_0, \alpha_0) = \int \mathcal{D}\tilde{q} e^{S_0(q, \tilde{q})} e^{-i \sum_{k=0}^N \tilde{q}_k \alpha_k r_k}, \quad (3)$$

where $\mathcal{D}\tilde{q} = \prod_{k=0}^N \frac{d\tilde{q}_k}{2\pi}$ and $S_0(q, \tilde{q})$ is the Martin-Siggia-Rose action of a diffusion process with drift [12], written in discretized form,

$$S_0(q, \tilde{q}) = i \sum_{k=0}^N \{ \tilde{q}_k (q_{k+1} - q_k - \tau N(q_k)) + i \frac{\tau D}{2} \tilde{q}_k^2 \}. \quad (4)$$

To further evaluate the expression for the path probability, let us assume that the r_k are Gaussian random variables with zero mean and variance $\langle r_k r_l \rangle = \tau Q \delta_{kl}$. After averaging with respect to the r_k we find

$$\begin{aligned} g_{N+1}(q_{N+1}; q_N, \alpha_N; \dots; q_0, \alpha_0) &= \\ \int \mathcal{D}\tilde{q} e^{i \sum_{k=0}^N \{ \tilde{q}_k (q_{k+1} - q_k - \tau N(q_k)) + \frac{i\tau(D+Q\alpha_k^2)}{2} \tilde{q}_k^2 \}} & \\ = \frac{1}{\sqrt{\prod_{k=0}^N 2\pi\tau(D+Q\alpha_k^2)}} e^{-\sum_{k=0}^N \frac{(q_{k+1}-q_k-N(q_k))^2}{2\tau(D+Q\alpha_k^2)}}. \end{aligned} \quad (5)$$

The probability density for a specific path $f_{N+1}(q_{N+1}; \dots; q_0)$ is then given by averaging with respect to the stochastic process α_k

$$f_{N+1}(q_{N+1}; \dots; q_0) = \int \mathcal{D}\tilde{q} e^{S_0(q, \tilde{q})} Z(i \frac{\tau Q}{2} \tilde{q}_N^2, \dots, i \frac{\tau Q}{2} \tilde{q}_0^2) \quad (6)$$

We have introduced the characteristic function

$$\begin{aligned} Z(\eta_N, \dots, \eta_0) &= \langle e^{i \sum_{k=0}^N \eta_k \beta_k} \rangle \\ &= \sum_{\alpha_N} \dots \sum_{\alpha_0} p(\alpha_N; \dots; \alpha_0) e^{i \sum_{k=0}^N \eta_k \alpha_k^2}. \end{aligned} \quad (7)$$

which is the characteristic function of the process $\beta_i = \alpha_i^2$. We have denoted the distribution of $\alpha = [\alpha_N, \dots, \alpha_0]$ by $p(\alpha)$.

Propagators: The representation (6) for the path probability serves as the starting point to determine propagators for the anomalous stochastic process defined by Eq.(1). As usual, the propagator is obtained by integration of all possible paths with appropriate boundary conditions

$$\mathcal{G}(q_N; q_0, N) = \int \mathcal{D}q f_N(q_N, \dots, q_1, q_0). \quad (8)$$

Let us consider a process consisting of two pure diffusions, i.e. we set $N(q_k) = 0$. We obtain

$$\mathcal{G}(q; q_0, N) = \sum_{\alpha} p(\alpha) \frac{e^{-\frac{(q-q_0)^2}{2\tau \sum_{k=0}^{N-1} [D+Q\alpha_k^2]}}}{\sqrt{2\pi\tau(\sum_{k=0}^{N-1} [D+Q\alpha_k^2])}}. \quad (9)$$

Observe that the quantity $S(N) = \sum_{k=0}^{N-1} \alpha_k^2$ plays a key role for the diffusion process. After introduction of the pdf $P_N(S) = \sum_{\alpha} p(\alpha) \delta_{S, \sum_{k=0}^{N-1} \alpha_k^2}$ we can rewrite Eq.(9) as

$$\mathcal{G}(q_N, q_0, N) = \sum_{S=0}^{\infty} P_N(S) \frac{e^{-\frac{(q-q_0)^2}{2\tau(ND+SQ)}}}{\sqrt{2\pi\tau(ND+SQ)}}. \quad (10)$$

In comparison to the regular diffusion process which takes place in the physical time $N\tau$ the second diffusion process can be interpreted to occur in the random time $S\tau$ whose distribution is determined by $p(\alpha)$. A corresponding result for a continuous jump-diffusion process was obtained in [13] with different methods.

Multiple-time propagators can be obtained from the propagators $\mathcal{G}(q_N, q_0, N)$ in a straightforward manner

$$\begin{aligned} \mathcal{G}(q_N, q_M, q_0) &= \sum_{S_N=0}^{\infty} \sum_{S_M=0}^{\infty} P_{N-M,M}(S_N - S_M; S_M) \\ &\times \mathcal{G}(q_N; q_M, N-M) \mathcal{G}(q_M; q_0, M). \end{aligned} \quad (11)$$

where $P_{N-M,M}(S_N - S_M; S_M)$ denotes the probability distribution of the variables $S_N - S_M = \sum_{k=M}^{N-1} \alpha_k^2$ and $S_M = \sum_{k=0}^{M-1} \alpha_k^2$, which can be evaluated using the probability distribution $p(\alpha)$. The generalization to n -time pdfs is straightforward and is given in terms of the pdf $P_{N-k,k-l,\dots,m}(S_N - S_k; S_k - S_l; \dots, S_m)$ and the product of the propagators $\mathcal{G}(q_N; q_M, M-N)$.

Examples for the α -process: All results obtained so far hold for a general process α . In the following we consider two specific examples for this process.

The case where the α_k are i.i.d. random variables with a common pdf $h(\alpha)$ is in the realm of superstatistics [11].

Renewal processes are obtained when the process α_k is a binary string. If we denote the number of zeros between two successive ones by t and assume them to be i.i.d. random variables with a common pdf $W(t)$, the process α is a renewal process. In this case the process described by Eq.(1) is a CTRW with internal dynamics [13, 14] which for $N(q_k) = D = 0$ includes the standard CTRW.

Path integrals for CTRWs: The starting point of our treatment of CTRW path integrals are Eqs. (6) and (7) and we need to characterize the process α . For the sake of simplicity, we restrict ourselves to processes with $\alpha_0 = 1$, i.e. processes that start with an event. The aim is to represent the probability of a specific sequence $p(\alpha)$ in terms of the waiting time distribution, i.e. the number of zeros between two successive ones. Let $W_{i,j}$ denote the probability to have $i-j-1$ zeros between ones at j and i , $i > j$ and let furthermore $W_{i,i} = 0$. It follows that the survival probability, i.e. the probability that a one at j is not followed by a further one till i is $1 - W_{i,j}$.

To proceed it is convenient to introduce the probability $\nu_k(1, \alpha_{k-1}, \dots, \alpha_1, 1)$ of truncated strings, $[1, 0, 0, \dots, 1, \dots, 0, 1]$ which end with the event at k . According to the definition of renewal processes the truncated densities fulfill the relation

$$\begin{aligned} \nu_k(1, \alpha_{k-1}, \dots, \alpha_1, 1) &= \delta_{k,0} \\ &+ \sum_{l=0}^k \sigma_{kl} \nu_l(1, \alpha_{l-1}, \dots, \alpha_1, 1), \end{aligned} \quad (12)$$

where we have defined

$$\sigma_{kl} = \delta_{\alpha_k, 1} \delta_{\alpha_{k-1}, 0} \dots \delta_{\alpha_{l+1}, 0} \delta_{\alpha_l, 1} W_{k,l}. \quad (13)$$

The density of the truncated strings for $k = N$ depends on the densities for $k < N$. Iterative application of (12) allows us to present the truncated density for $k = N$

according to

$$\begin{aligned} \nu_N(1, \alpha_{k-1}, \dots, \alpha_1, 1) = \\ \sigma_{N0} + \sum_{l=0}^N \sigma_{Nl} \sigma_{l0} + \sum_{l=0}^N \sum_{l'=0}^l \sigma_{Nl} \sigma_{ll'} \sigma_{l'0} + \dots \\ \dots + \sigma_{NN-1} \sigma_{N-1N-2} \dots \sigma_{21} \sigma_{10}, \end{aligned} \quad (14)$$

where $N > l > l' > \dots > 0$. This series can be summed, yielding

$$\nu_k(1, \alpha_{k-1}, \dots, \alpha_1, 1) = \sum_{l=0}^N [E - \sigma]_{kl}^{(-1)} \sigma_{l0}, \quad (15)$$

where E denotes the unit matrix and σ is a matrix with elements σ_{ij} . Relation (15) is valid for $k \leq N$ and implies that the truncated densities are defined by a Dyson equation whose explicit solution is given by matrix inversion of $E - \sigma$.

The probability density $p(\alpha_N, \dots, \alpha_0)$ of the renewal process then is determined from the truncated densities on the basis of the relationship

$$p(\alpha_N, \dots, \alpha_0) = \sum_{l=0}^N \gamma_{Nl} \nu_l(1, \alpha_{l-1}, \dots, \alpha_1, 1), \quad (16)$$

where we have defined

$$\gamma_{Nl} = \delta_{\alpha_N, 1} \delta_{N, l} + (1 - W_{Nl}) \delta_{\alpha_N, 0} \delta_{\alpha_{N-1}, 0} \dots \delta_{\alpha_{l+1}, 0} \delta_{\alpha_l, 1}. \quad (17)$$

The explicit representation of the probability density is then just

$$p(\alpha_N, \dots, \alpha_0) = \sum_{k=0}^N \sum_{l=0}^N \gamma_{Nk} [E - \sigma]_{kl}^{(-1)} \sigma_{l0}. \quad (18)$$

Again, an expansion of the matrix $[E - \sigma]^{-1}$ yields a representation of the probability density of a string $[0, \dots, 1, \dots, 1]$ in the number of one's contained in the string. Concluding, we state the characteristic function of the renewal process α which can be easily assessed on basis of Eq.(18):

$$Z(\eta_N, \dots, \eta_0) = \sum_{k=0}^N \sum_{l=0}^N \tilde{\gamma}_{Nk} [E - \tilde{\sigma}]_{kl}^{(-1)} \tilde{\sigma}_{l0}, \quad (19)$$

where now

$$\tilde{\gamma}_{kl} = (1 - W_{kl}) e^{i\eta_l}, \quad \tilde{\sigma}_{kl} = e^{i\eta_k} W_{kl} e^{i\eta_l}. \quad (20)$$

The combination of Eq.(7) with Eq.(19) provides the desired path-integral representation for the class of CTRWs under consideration.

Since this path-integral representation is a rather condensed representation of the CTRW we proceed to derive a more transparent formulation. It is based on Eqs. (12) and (18). It is clear, that the probability

distribution $f_{N+1}(q_{N+1}, q_N, \dots, q_0)$ should have an analogous representation. We introduce the abbreviations $K_0(q_N; \dots, q_1)$ for the path probability of the MSR action (4) and $V(q_{l+1}; q_l)$ for the short time propagator of the action with $\alpha_l = 1$

$$V(q_{l+1}; q_l) = \frac{1}{\sqrt{2\pi\tau(D+Q)}} e^{-\frac{(q_{l+1} - q_l - N(q_l))^2}{2\tau(D+Q)}}. \quad (21)$$

The starting point is the definition of the truncated distribution

$$\begin{aligned} \eta_N(q_{N+1}, q_N, \dots, q_0) = \sum_{\alpha} \nu_N(1, \alpha_{N-1}, \dots, \alpha_1, 1) \\ \times g_{N+1}(q_{N+1}; q_N, 1; q_{N-1}, \alpha_{N-1}; \dots; q_0, 1). \end{aligned} \quad (22)$$

Using the relation (12) we arrive at the Dyson equation for the truncated distribution

$$\begin{aligned} \eta_k(q_{k+1}, q_k, \dots, q_0) = \delta_{k,0} V(q_1, q_0) \\ + \sum_{l=0}^k V(q_{k+1}, q_k) W_{kl} K_0(q_k, \dots, q_{l+1}) \eta_l(q_{l+1}, \dots, q_0). \end{aligned} \quad (23)$$

Employing Eq.(16) we can establish the connection between the distributions η and f :

$$\begin{aligned} f_{N+1}(q_{N+1}, q_N, \dots, q_0) = \\ \sum_{l=0}^N (1 - W_{Nl}) K_0(q_{N+1}, \dots, q_{l+1}) \eta_l(q_{l+1}, \dots, q_0). \end{aligned} \quad (24)$$

The relations (23) and (24) yields a representation of the path-probability of the CTRW in terms of K_0 and V . As we will show below, this representation can be the starting for determining expectation values of the path.

It is possible to combine both equations, (23) and (24) to obtain the representation of the joint probability distribution as

$$\begin{aligned} f_{N+1}(q_{N+1}, q_N, \dots, q_0) = \sum_{l=0}^N (1 - W_{Nl}) K_0(q_{N+1}, \dots, q_{l+1}) \\ [\delta_{lk} - V(q_{l+1}, q_l) W_{lk} K_0(q_l, \dots, q_{k+1})]^{(-1)} V(q_1, q_0) \delta_{k,0}. \end{aligned} \quad (25)$$

Thereby, the Dyson equation (23) was solved explicitly.

Expansion of the inverse matrix then yields an expansion of the path probability in terms of the number of events. The first term $f^{(0)}$ yields the contribution of paths during which no event occurred after the first.

$$f_{N+1}^{(0)}(q_{N+1}; \dots; q_0) = (1 - W_{N,0}) K_0(q_{N+1}; \dots; q_1) V(q_1; q_0), \quad (26)$$

whereas the first order term contains the contribution from paths with one event

$$\begin{aligned} f_{N+1}^{(1)}(q_{N+1}; \dots; q_0) = \sum_{l=1}^N (1 - W_{N,l}) \times \\ K_0(q_{N+1}; \dots; q_{l+1}) V(q_{l+1}; q_l) W_{l,0} K_0(q_l; \dots; q_1) V(q_1; q_0). \end{aligned} \quad (27)$$

Higher order terms are obtained in the same way. Note the formal analogy to the self-energy corrections in quantum theory. In this case the corrections to the free propagator are given by the anomalous contributions from the α -process. By considering processes which start with an event, we imply non-equilibrium conditions. Relaxing this condition would lead to the case of aging CTRWs [15].

Generalized Fokker-Planck Equation and Generalized Feynman-Kac Formula: We want to conclude with the derivation of the generalized Fokker-Planck equation for the CTRW-case. Apparently, we can also derive Feynman-Kac formulas [16]. Let us consider the functional

$$P_{N+1}(p, q_{N+1}) = \int \prod_{j=0}^N dq_j e^{ip \sum_{k=0}^N U(q_k)} f_{N+1}(q_{N+1}, \dots, q_0). \quad (28)$$

The quantity $P_{N+1}(0, q_{N+1})$ is just the probability distribution $f_{N+1}(q_{N+1})$ which obeys a generalized Fokker-Planck equation. Defining now

$$G(q_{N+1}, q_l; p, N, l) = \int \prod_{j=l+1}^N dq_j e^{ip \sum_{k=l+1}^N U(q_k)} f_{N+1-l}(q_{N+1}, \dots, q_l), \quad (29)$$

as well as

$$\zeta_l(p, q_{l+1}) = \int \prod_{j=0}^{l+1} dq_j e^{ip \sum_{k=0}^l U(q_k)} \eta_l(q_{l+1}, \dots, q_0), \quad (30)$$

we obtain from from Eqs. (23) and (24) the relations

$$P_{N+1}(p, q_{N+1}) = \sum_{k=0}^N (1 - W_{N,k}) \times \int dq_{k+1} G(q_{N+1}, q_{k+1}; p, N, k) \zeta_l(p, q_{k+1}), \quad (31)$$

$$\zeta_k(p, q_{k+1}) = V(q_1, q_0) \delta_{l,0} + \sum_{l=0}^k \int dq_k \int dq_{l+1} V(q_{k+1}, q_k) W_{k,l} G(q_k, q_{l+1}, k, l+1) \zeta_l(p, q_{l+1}). \quad (32)$$

Now Eqs. (31) and (32) are just the time-discrete versions of the equations which served as the starting point for the derivation of generalized Fokker-Planck equation for the CTRW with internal dynamics [13] eventually leading to

$$\left[\frac{\partial}{\partial t} - \mathcal{H} \right] P(p, q, t) = \int_0^t dt' Q(t-t') \mathcal{L}_1 e^{(t-t')\mathcal{H}} P(p, q, t'), \quad (33)$$

where $\mathcal{H} = \mathcal{L}_0 + ipU(q)$. \mathcal{L}_0 is the generator of the Fokker-Planck process with $\alpha = 0$ and $Q(t-t')$ is the common time-evolution kernel of CTRWs [6]. For the case of CTRWs without internal dynamics, i.e. $\mathcal{L}_0 = 0$, this equation was recently derived in [17].

Conclusions and Outlook In summary, we have presented the path integral formulation for a class of generalized diffusion processes which includes the CTRW. Applying the path integral, we have derived general expressions for the propagators and the multipoint distributions. For the case of CTRW-processes we found a closed form expression for the probability density of a path in terms of the waiting time distribution. We expect that this expression will help to evaluate interesting functionals for anomalous diffusion processes. Furthermore, we want to mention that it is tempting to consider the case, where the renewal process α is generated by a one-dimensional map [18], along similar lines.

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- [1] F. Langouche, D. Roekaerts and E. Tirapegui, *Functional Integration and Semiclassical Expansions* (Reidel, Dordrecht, The Netherlands, 1982).
 - [2] H. Kleinert *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics and Financial Markets* (World Scientific, Singapore, 2009).
 - [3] L. Onsager and S. Machlup, Phys. Rev. **91**, 1505 (1953).
 - [4] H. Haken, Z. Phys. B **24**, 321 (1976); R. Graham, Z. Phys. B **26**, 281 (1977); P. Hänggi Z. Physik B **75**, 275 (1989).
 - [5] J.P. Bouchaud and A. Georges, Phys. Rep. **195**, 127 (1990).
 - [6] R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000); R. Metzler and J. Klafter, J. Phys. A:Math. Gen. **37**, R161 (2004).
 - [7] M.F. Shlesinger, G.M. Zaslavsky and J. Klafter, Nature **363**, 31 (1993).
 - [8] E. Montroll and G.H. Weiss, J. Math. Phys **6**, 167 (1965).
 - [9] H.C. Fogedby, Phys. Rev. E **50**, 1657 (1994); S. Eule and R. Friedrich, EPL **86**, 30008 (2009).
 - [10] A. Baule and R. Friedrich, Phys. Rev. E **71**, 026101 (2005).
 - [11] C. Beck and E.G.D. Cohen, Physica A **322**, 267 (2003).
 - [12] P.C. Martin, E.D. Siggia and H.A. Rose, Phys. Rev. A **8**, 423 (1973); B. Shraiman, C.E. Wayne and P.C. Martin, Phys. Rev. Lett. **46**, 935 (1981).
 - [13] S. Eule, R. Friedrich, F. Jenko and I. Sokolov, Phys. Rev. E **78**, 060102(R) (2008).
 - [14] R. Friedrich, F. Jenko, A. Baule and S. Eule, Phys. Rev. Lett. **96**, 230601 (2006).
 - [15] E. Barkai and Y.-C. Cheng, J. Chem. Phys. **118**, 6167 (2003).

- [16] S.N. Majumdar, Curr. Sci. **89**, 2076 (2005).
- [17] L. Turgeman, S. Carmi and E. Barkai, Phys. Rev. Lett. **103**, 190201 (2009); S. Carmi, L. Turgeman and E. Barkai, J. Stat. Phys. **141**, 1071 (2010).
- [18] T. Geisel and S. Thomae, Phys Rev. Lett. **52**, 1963 (1984); G. Zumofen and J. Klafter, Phys. Rev. E **47**, 851 (1993).